Small Business Innovation Research

# Human-Machine-Task Computer Aided Design Software

Moldyn Inc./Photon Research Associates, Inc. Cambridge, MA



#### INNOVATION

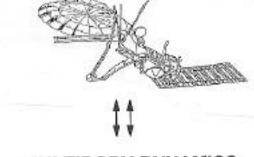
Very fast Order (N) algorithm for simulating biomechanical motion, spacecraft, vehicle and machine dynamics, and complex macromolecules dynamics

#### **ACCOMPLISHMENTS**

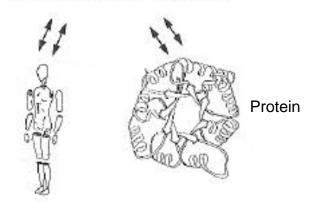
- Developed macromolecular version Multibody Order (N) Dynamics (MBO(N)D) using internal funds and a \$2M Phase III grant from NIST/ATP funds.
- Achieved 100 times speedup in processing molecular dynamics.
- Breakthrough solving equations used in simulating large molecules over long periods of time.

#### COMMERCIALIZATION

- Commercial potential in drug design was far greater than the original application of man machine interaction dynamics and performance analysis tool.
- Commercial release of MBO(N)D code for Spring 1998 through partner, Molecular Simulations, Inc., a major world-wide computational chemistry software retailer.
- 1998 estimated sales \$2M.



### MULTIBODY DYNAMICS



## **GOVERNMENT/SCIENCE APPLICATIONS**

- Innovative polymers, composites for aerospace of interest to NASA Langley Research Center and DoD
- Biochemical molecules for sensing and computation DoD
- Nanostructured materials of interest to NASA Ames Research Center, DoD, and DOE
- Drugs for public health and military needs NIH, & DoD

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